

2-Aminobenzoic acid, ethoxycarbonylated, TBDMS

Inchi:	InChI=1S/C16H25NO4Si/c1-7-20-15(19)17-13-11-9-8-10-12(13)14(18)21-22(5,6)16(2,3)
InchiKey:	UKDXDHTZAGVJFG-UHFFFAOYSA-N
Formula:	C16H25NO4Si
SMILES:	CCOC(=O)Nc1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	323.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	4.417		Crippen Method
rinpol	2072.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R562960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/53-872-5/2-Aminobenzoic-acid-ethoxycarbonylated-TBDMS.pdf>

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